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MOLECULAR STATICS SIMULATION OF DISLOCATION PILEUP USING QUASICONTINUUM METHOD

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Abstract: *In this contribution, accuracy of the QuasiContinuum (QC) methodology is studied for the case of dislocation pileup against an impenetrable obstacle in two-dimensional hexagonal lattices. To this end, a simplified shear test with a predetermined horizontal glide plane and next-to-nearest interactions described by the Lennard-Jones potential is adopted. The full molecular statics solution is computed, which is compared to two different QC simulations in terms of spatial positioning of individual dislocations along the glide plane, corresponding disregistry profiles, and dislocation core structures.*

Keywords: atomistic simulation, molecular statics, QuasiContinuum, dislocation pileup

1. Introduction

Dislocations are the determining factor for material behavior such as plastic slip or crack initiation, which are one of the most common reasons of material failure. Numerical simulation of dislocations therefore play an important role across many engineering fields. Simulation of dislocations on the atomistic level is the most accurate approach, but requires large computational costs that limit its applicability. In order to decrease the computational cost, several models that use different scales have been introduced in the literature, such as discrete-to-continuous methods, continuous Peierls–Nabarro models, discrete dislocation method, or dislocation density models.

In this work, molecular statics is used to model dislocation pileup in two-dimensional hexagonal lattices. Quasicontinuum methodology is employed to reduce the excessive computational costs, and its accuracy and efficiency is compared against the full atomistic model.

2. Full atomistic model

Atomistic models in molecular statics are characterized by an underlying lattice and interatomic potential. In this work, hexagonal lattices are adopted with interactions described by the Lennard-Jones (LJ) potential

$$\phi^{\alpha\beta}(r^{\alpha\beta}) = \varepsilon \left[\left(\frac{r_{\mathrm{m}}}{r^{\alpha\beta}} \right)^{12} - 2 \left(\frac{r_{\mathrm{m}}}{r^{\alpha\beta}} \right)^{6} \right]. \tag{1}$$

In Eq. (1), $r^{\alpha\beta} = ||\boldsymbol{r}^{\beta} - \boldsymbol{r}^{\alpha}||_{\ell^2}$ denotes the distance between two atoms α and β positioned at $\boldsymbol{r}^{\alpha}$ and $\boldsymbol{r}^{\beta}$, ε is the depth of the energy well, and r_m denotes the distance at which the interaction energy reaches its minimum, cf. Fig. 1 (left). The total potential energy of an atomic structure is evaluated as a sum over all interactions, i.e.

$$E = \frac{1}{2} \sum_{\alpha,\beta;\ \alpha \neq \beta}^{N^{\mathrm{Atm}}} \phi^{\alpha\beta}(r^{\alpha\beta}). \tag{2}$$

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Because evaluation of the interatomic potential for all pairwise combinations is expensive, and because long-distance interactions have negligible contributions to the total potential energy (cf. Fig. 1 left), only interactions within the so-called *cutting radius*, r_{cut}, are usually considered. Such a simplification introduces a discontinuity in $\phi^{\alpha\beta}(r_{cut})$, which is removed by subtracting a linear function to yield zero value and zero slope at $r^{\alpha\beta} = r_{cut}$.

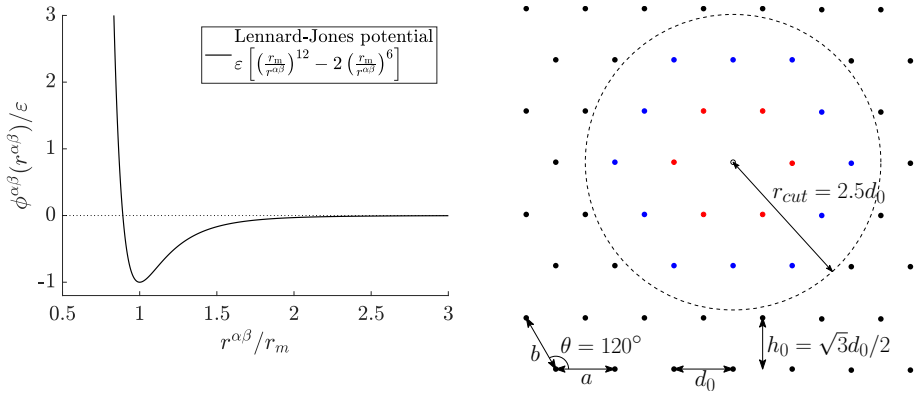

Fig. 1: Lennard-Jones potential (left), and two-dimensional hexagonal lattice (right). Considered atom (empty circle), its nearest neighbors (red dots), next-to-nearest neighbors (blue dots), and the remaining atoms situated outside the cutting radius (black dots).

Adopted hexagonal lattice has a lattice spacing d_0, meaning that the cutting radius $r_{cut} = 2.5\, d_0$ provides next-to-nearest interactions (shown in Fig. 1 right). In order to find a stress-free configuration, initial relaxation is carried out for the ideal lattice with periodic boundary conditions and initial lattice spacing $d_0 = r_m$, which results in a hexagonal lattice with a slightly adjusted lattice spacing $d_0 = 0.9917496\, r_m$. This updated value of d_0 is used as the initial lattice spacing for all simulations listed below.

At each time step, corresponding boundary conditions (prescribed displacements) are incremented, yielding an imbalanced system. Equlibration is carried out using the trust-region algorithm, which provides updated positions of all atoms $\boldsymbol{r}$ that minimize E. The resulting configuration is stored and used as the initial guess in the next time step.

3. Quasicontinuum

Quasicontinuum (QC) methodology is a concurrent multiscale technique originally introduced by Tadmor et al. (1996). The key idea of the QC is that it combines accurate but expensive atomistic description where needed with relatively cheap continuum approximation elsewhere. Considered domain is therefore divided into two parts; in the fully refined region, the full atomistic system is resolved exactly, whereas in the coarse-grained region (triangular) interpolation elements are introduced, yielding effectively a continuum approximation. Only the nodes of adopted triangulation are considered to describe the kinematics of the entire system. They are called representative atoms, or *repatoms* for short, and their positions are stored in a column $\boldsymbol{r}_{rep}$. High number of degrees of freedom (DOFs) associated with the full system is thereby significantly reduced, whereas positions of all atoms $\boldsymbol{r}$ can be obtained by *interpolation*, i.e.

$$\boldsymbol{r} = \boldsymbol{\Phi}\boldsymbol{r}_{rep}. \tag{3}$$

In Eq. (3), $\boldsymbol{\Phi}$ denotes an interpolation matrix associated with adopted triangulation.

In the next step, *summation* rule is introduced to approximately evaluate the total potential energy of the entire system. Site energies of all interpolated atoms situated inside one triangular element can be approximated by the energy of a few, or even only one *sampling atom* with its corresponding weight factor w_α. The total energy can be then estimated as

$$E = \sum_{\alpha}^{N^{\mathrm{SampAtm}}} w_\alpha \phi_\alpha \quad \text{with} \quad \phi_\alpha = \frac{1}{2} \sum_{\substack{\beta;\ \alpha\neq\beta \\ r^{\alpha\beta}<r_{cut}}}^{N^{\mathrm{Atm}}} \phi^{\alpha\beta}(r^{\alpha\beta}), \tag{4}$$

Tab. 1: Properties of different models

	Atoms	Reaptoms	Sampling atoms	Elements	Unknown DOFs	Newton iterations	Solving time
Full model	65 921	-	-	-	128 632	3 381	1.0
QC1	65 921	6 967	10 317	3 043	12 449	2 738	0.105
QC2	65 921	16 961	20 209	2 954	32 437	3 194	0.243

where ϕ_α is the site energy of a sampling atom α. Several possible ways exist to select appropriate sampling atoms. The central summation rule after Beex et al. (2014) is used throughout this work.

Note finally that the fully-refined regions and used interpolation mesh can adaptively change at each iteration or time increment in order to increase the accuracy, or to capture movement of individual dislocations. In this contribution, however, only a fixed triangulation is considered for simplicity.

4. Results

A simplified shear example is adopted to analyze dislocations propagating along a predetermined glide plane, geometry of which is sketched in Fig. 2 (left). Shear opening of the notch is governed by prescribed horizontal displacements along the left vertical edge. The prescribed displacement $\bar{u}$ is increased to its final value $5\,d_0$ in 100 uniform loading steps. For such a type of loading, dislocations are expected to propagate along the horizontal glide plane positioned in the mid-height of the specimen. In QC simulations, fully resolved region is situated in the close vicinity of the glide plane, using two different meshes. In the first case (abbreviated as QC1), the height of the fully refined region is $16\,h_0$, cf. Fig. 2 (right). In the second case (abbreviated as QC2), the height is chosen as $64\,h_0$. Corresponding numerical properties of all three models are summarized in Table 1.

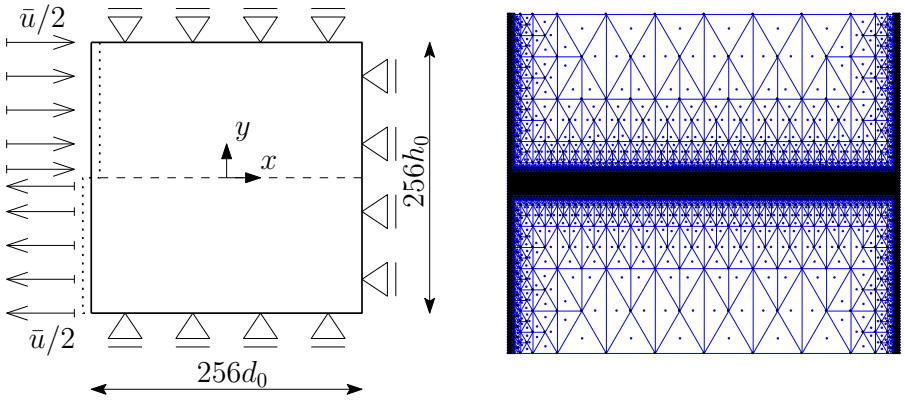

Fig. 2: (left) A sketch of the shear example used in simulations along with its deformed shape (dotted line), and corresponding glide plane (dashed line). (right) Triangulation of adopted model QC1; repatoms are shown as black dots, interpolation elements as blue triangles, and sampling atoms as blue dots.

Obtained QC results are next compared against the full atomistic simulation. Disregistry and opening profiles are depicted in Fig. 3 (left), whereas positions of individual dislocations in different loading steps are compared in Fig. 3 (right). Although all simulations provide generally very similar results, it is worth noting that in the full simulation, the dislocations propagate mainly in small jumps, whereas in QC1 the propagation of dislocations seems to be smoother, cf. Fig. 3 (right). This difference is observed mainly for the dislocations located closer to the right edge, where the influence of the impenetrable obstacle is strongest. This kind of behavior can be explained by different dislocation core structures. For QC1, the height of the fully resolved region is not sufficient, yielding a distorted shape of the dislocation core shown

in Fig. 4 (right). Distorted dislocation cores observed in QC solutions have a smoother disregistry profile (Fig. 3 left inset), and they are less stable. Such dislocations propagate more easily and slightly further when compared to the full solution. The solution corresponding to the QC2 system on the other hand provides the correct shape of the dislocation core structure and hence, the positioning of individual dislocations is more accurate in this case, see Fig. 3 (left).

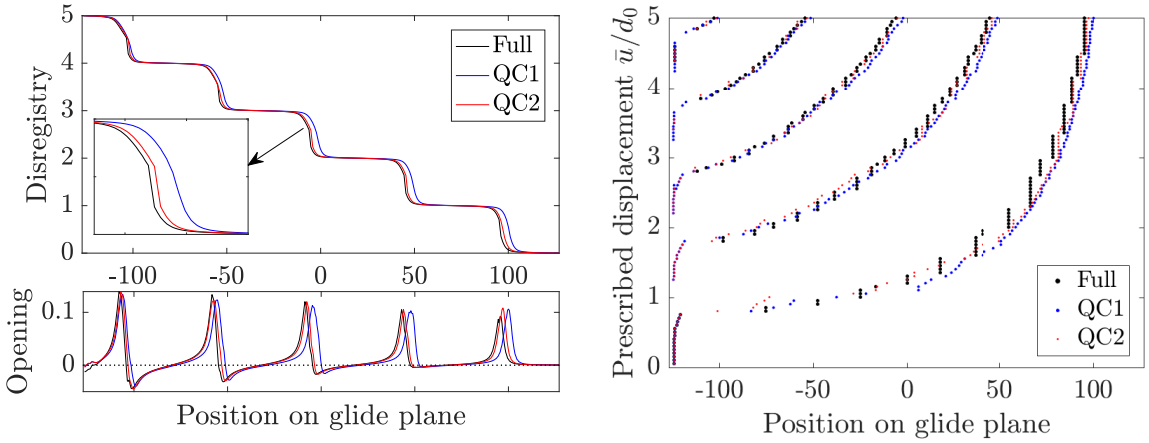

Fig. 3: Disregistry profile (left top) and opening profile (left bottom) normalized by the lattice spacing d_0. Positioning of individual dislocations as a function of the external loading (right).

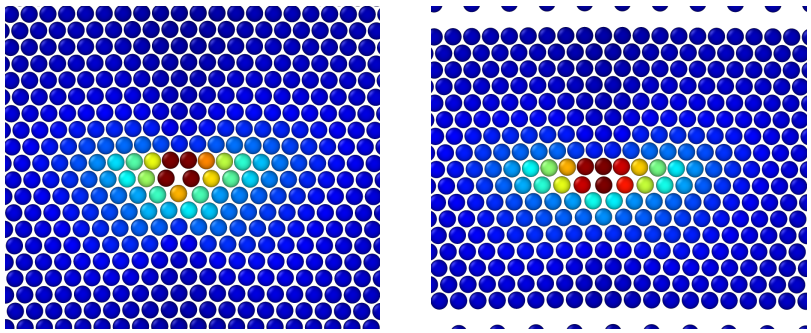

Fig. 4: Dislocation core structures corresponding to the full model (left), and to the QC1 model (right). Coloring of individual atoms reflects the level of local lattice disregistry (increasing from blue to red).

5. Conclusions

In this contribution, a comparison of the QC model against the full molecular statics solution for the case of dislocation pileup in two-dimensional hexagonal lattices has been provided. It has been shown that the QC system is rather sensitive to the choice of triangulation, but provides significant computational savings.

Acknowledgments

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